Two remarks on the local Hamiltonian problem*

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Abstract

In this note we present two natural restrictions of the local Hamiltonian problem which are BQP-complete under Karp reduction. Restrictions complete for QCMA, QMA_1, and MA were demonstrated previously.

Introduction. The complexity class BQP captures those problems solvable in polynomial time by bounded-error quantum algorithms. BQP has complete "promise problems" – for example, determining the sign of a quadratically signed weight enumerator [12], obtaining additive approximations to the Jones polynomial [5] and the Tutte polynomial [3] evaluated at specific points, estimating the diagonal entries of a matrix power [10], and sampling from the energy eigenvalues of a local Hamiltonian [15].

In this note we demonstrate two promise problems which are (a) BQP-complete under *Karp reduction*, or polynomial-time transformation, and (b) natural restrictions of the canonical QMA-complete "local Hamiltonian problem" [11] likely to arise in computational physics applications. Our observations are in the spirit of results [14, 7, 8] which demonstrated restrictions of the local Hamiltonian problem complete for QCMA, QMA_1 and MA.

Definitions. A *promise problem* P is the disjoint union of two sets $L_0, L_1 \subseteq \{0,1\}^*$. A bounded-error algorithm A *decides* P if its output bit $A(x)$ satisfies:

$$x \in L_b \Rightarrow \Pr[A(x) = b] \geq 2/3 \tag{1}$$

Inputs $x \notin L_0 \cup L_1$ are "promised" not to occur; equivalently, they can cause A to behave arbitrarily. If A is a quantum (resp., classical) algorithm running in time $O(poly(|x|))$, then P is in BQP (resp., BPP). A BQP *verifier* V takes both an input $x \in L_0 \cup L_1$ and a quantum *witness* state $|\psi\rangle$ on $O(poly(|x|))$ qubits and outputs a bit $V(x, |\psi\rangle)$ satisfying:

$$x \in L_1 \quad \Rightarrow \quad \exists |\psi\rangle \;:\; \Pr[V(x, |\psi\rangle) = 1] \geq 2/3 \tag{2}$$

$$x \in L_0 \quad \Rightarrow \quad \forall |\psi\rangle \;:\; \Pr[V(x, |\psi\rangle) = 1] \leq 1/3 \tag{3}$$

If there is a BQP verifier for P, then P is in QMA. We obtain the complexity class (a) QMA_1 by changing the completeness parameter in line (2) from 2/3 to 1, (b) QCMA by restricting the (witness, verifier) pair to be (classical, quantum), (c) MA by restricting the pair to be (classical, classical), and (d) NP by restricting the pair to be (classical, classical) and changing the soundness parameter in line (3) from 1/3 to 0.

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Let $G = (V, E)$ be a hypergraph whose n vertices are d-state spins ("qudits" with d-dimensional Hilbert space $\mathcal{H}_d$) and whose hyperedges are k-subsets of qudits. We shall assume that d and k are fixed independently of the scaling parameter n. Denote by $H_e : \mathcal{H}_d^{\otimes k} \to \mathcal{H}_d^{\otimes k}$ a Hamiltonian (Hermitian operator) acting on the qudits $e \in E$, and let I be the identity operator. A *k-local Hamiltonian* has the form:

$$H = \sum_{e \in E} H_e \otimes I_{V \setminus e} \tag{4}$$

Its *ground state energy* is its minimum eigenvalue λ_1, and an eigenvector with eigenvalue λ_1 is a *ground state*. The *local Hamiltonian problem* (LH-MIN) is to decide if λ_1 is at most a ("YES") or at least $b = a + \Delta$ ("NO"), where $\Delta = \Omega(1/poly(n))$ is the *promise gap* and λ_1 is promised not to lie in (a, b). The inequality $\lambda_1 \leq a$ can be demonstrated by verifying the existence of a *low-energy state* for H – i.e., a state $|\psi\rangle$ satisfying $\langle\psi|H|\psi\rangle \leq a$. LH-MIN is QMA-complete by Kitaev [11].

A low-energy state promise. Let $U = U_L \cdots U_2 U_1$ be an n-qubit, L-gate BQP circuit with input $x \in L_b$ (hardwired into the first few gates) that maps the classical bitstring $|00\cdots 0\rangle$ to a quantum state whose "answer qubit" outputs b with probability at least 2/3 when measured. Using known techniques [11, 6] it is straightforward to build from U a local Hamiltonian

$$H = H_{in} + H_{prop} + H_{clock} + H_{out} \tag{5}$$

on n "circuit" qubits and L "clock" qubits such that (i) the terms H_{in}, H_{prop}, and H_{clock} ensure that any low-energy state of H encodes the circuit computation $U|00\cdots 0\rangle$ and accompanying clock ticks $|1^l 0^{L-l}\rangle \mapsto |1^{l+1} 0^{L-(l+1)}\rangle$ correctly, and (ii) the final term H_{out} ensures that any low-energy state of H corresponds to an input $x \in L_1$. More precisely, there exist parameters $a < b$ with $\Delta = b - a = \Omega(1/poly(n))$ such that (a) if $x \in L_0$ then every state $|\psi\rangle$ has energy $\langle\psi|H|\psi\rangle \geq b$, and (b) if $x \in L_1$ then the state

$$|\eta\rangle := \frac{1}{\sqrt{L+1}} \sum_{l=0}^{L} U_l \cdots U_1 |00\cdots 0\rangle \otimes |1^l 0^{L-l}\rangle \tag{6}$$

has energy $\langle\eta|H|\eta\rangle \leq a$. Notice that $|\langle 00\cdots 0|\eta\rangle|^2 \geq \frac{1}{L+1} = \Omega(1/poly(n))$. Thus, we have demonstrated a Karp reduction from an arbitrary promise problem in BQP to a special case of LH-MIN (let us call it LH-MIN*) in which every YES instance H possesses a low-energy state $|\psi\rangle = |\eta\rangle$ of "large" (i.e., size $\Omega(1/poly(n))$) inner product with an *a priori* known classical state – the bitstring $|00\cdots 0\rangle$ in this case, but we could just as easily have chosen any classical bitstring. Furthermore, LH-MIN* can be solved in BQP using the Abrams-Lloyd algorithm [2] (phase estimation on e^{iH}) with $|00\cdots 0\rangle$ as the input state. Thus, we have:

Remark 1 *The promise problem LH-MIN* is BQP-complete under Karp reduction.*

The promise on YES instances of LH-MIN* is a natural one and might be efficiently verifiable for typical inputs using perturbation theory. The related problem of *sampling* an eigenvalue λ_k of H from the distribution $|\langle x|\phi_k\rangle|^2$, where $|\phi_k\rangle$ is the eigenvector for λ_k and $|x\rangle$ is a classical bitstring, is BQP-complete under *Cook reduction* – i.e., an oracle for the problem can be used by a BPP machine to solve any problem in BQP [15].

Consider the problem obtained by modifying LH-MIN* so that for a YES instance, the classical state of large inner product with a low-energy state $|\psi\rangle$ is no longer $|00\cdots 0\rangle$, but rather some

unknown classical state $|b_1 b_2 \cdots b_n\rangle$. Without modification, Kitaev's QMA-completeness theorem for LH-MIN [11] shows that this problem is QCMA-complete. The problem remains in QCMA if for a YES instance, H is required only to have a low-energy state $|\psi\rangle$ of large (size $\Omega(1/poly(n))$) inner product with some state $|\psi'\rangle$ computable by a polynomial-size quantum circuit (cf. [14]): given the circuit's description as a witness, the verifier can prepare $|\psi'\rangle$ and then run Abrams-Lloyd.[1] Similarly, our BQP-complete problem LH-MIN* remains so if the state approximating $|\psi\rangle$ is relaxed from a known classical state to a quantum state having a known polynomial-time construction.

A spectral gap promise. Estimating the ground state energy of a local Hamiltonian H is a central one in computational physics. In practice, when the *spectral gap* $\delta := \min_{k \neq 1} \lambda_k - \lambda_1$ of H is large, the problem is often solvable efficiently by a classical divide-and-conquer "renormalization group" algorithm. Nevertheless, our argument that LH-MIN* is BQP-complete implies that even its "gapped" version is unlikely to have an efficient classical algorithm: the Hamiltonian

$$H' = H_{in} + H_{prop} + H_{clock} \tag{7}$$

has a spectral gap $\delta' = \Omega(1/poly(n))$ above its *unique* (non-degenerate) ground state $|\eta\rangle$ [11, 6], so we can choose the perturbation H_{out} both (a) large enough so that the promise gap Δ for λ_1 is $\Omega(1/poly(n))$ and (b) small enough so that the spectral gap δ of H is $\Omega(1/poly(n))$ just like that of H'.[2] At this point, we may reparametrize $(a, b) \mapsto (a, a + \delta)$ to conclude that the special case of LH-MIN* which for a YES instance has a unique eigenvalue at most a and every other eigenvalue at least b (let us call this problem UNIQUE-LH-MIN*) remains BQP-complete:

Remark 2 *The promise problem UNIQUE-LH-MIN* is BQP-complete under Karp reduction.*

Now consider the problem obtained by modifying UNIQUE-LH-MIN* so that for a YES instance, the classical state of large inner product with a low-energy state $|\psi\rangle$ is an unknown classical state $|b_1 b_2 \cdots b_n\rangle$. We might guess that it is QCMA-complete, and this is essentially true: although the Karp reduction given by Kitaev [11] does not produce a gapped H if there are multiple classical witnesses, we can force it to do so by composing it with a randomized reduction of the sort used by Valiant and Vazirani [13].

Interestingly, it is not known how to apply the Valiant-Vazirani technique to H if its eigenvectors (as an unordered set of orthogonal axes) are unknown and highly non-classical [4]. Perhaps it is not possible: there is some theoretical evidence that a large spectral gap implies that the ground state exhibits little long-range entanglement [9] and is therefore approximable by a succinct (classical) representation such as a "matrix product state." If this were true generally, then one could not reduce LH-MIN to gapped instances without also showing QMA=QCMA.

Further directions. Beyond those we have already mentioned, there are several LH-MIN restrictions known to be complete for various subclasses of QMA: If we restrict the local terms H_e of H to be classical (i.e., diagonal), we obtain an NP-complete problem generalizing MAX-k-SAT. If we restrict each H_e to be a projection matrix and set $a = 0$, we obtain the "quantum k-SAT" problem complete for QMA_1 [7]. If these projection matrices are required to have nonnegative entries, we

[1] The space of quantum states is too large to cover with such a fine ϵ-net using circuits of only polynomial size; otherwise, it would trivially follow that QCMA=QMA [1].

[2] This choice guarantees for both YES *and* NO instances that the spectral gap above the ground state is large, although we ignore the latter property henceforth.

obtain the "stoquastic k-SAT" problem complete for MA [8]. Determining the degree to which each of these promise problems can be relaxed or tightened while retaining the same computational complexity merits further investigation.

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